Finite Element Model Characterization Of Nano-Composite Thermal And Environmental Barrier Coatings

Thermal and environmental barrier coatings have been applied for protecting Si based ceramic matrix composite components from high temperature environment in advanced gas turbine engines. It has been found that the delamination and lifetime of T/EBC systems generally depend on the initiation and propagation of surface cracks induced by the axial mechanical load in addition to severe thermal loads. In order to prevent T/EBC systems from surface cracking and subsequent delamination due to mechanical and thermal stresses, T/EBC systems reinforced with nano-composite architectures have showed promise to improve mechanical properties and provide a potential crack shielding mechanism such as crack bridging. In this study, a finite element model (FEM) was established to understand the potential beneficial effects of nano-compsoites systems such as SiC nanotube-reinforced oxide T/EBC systems.

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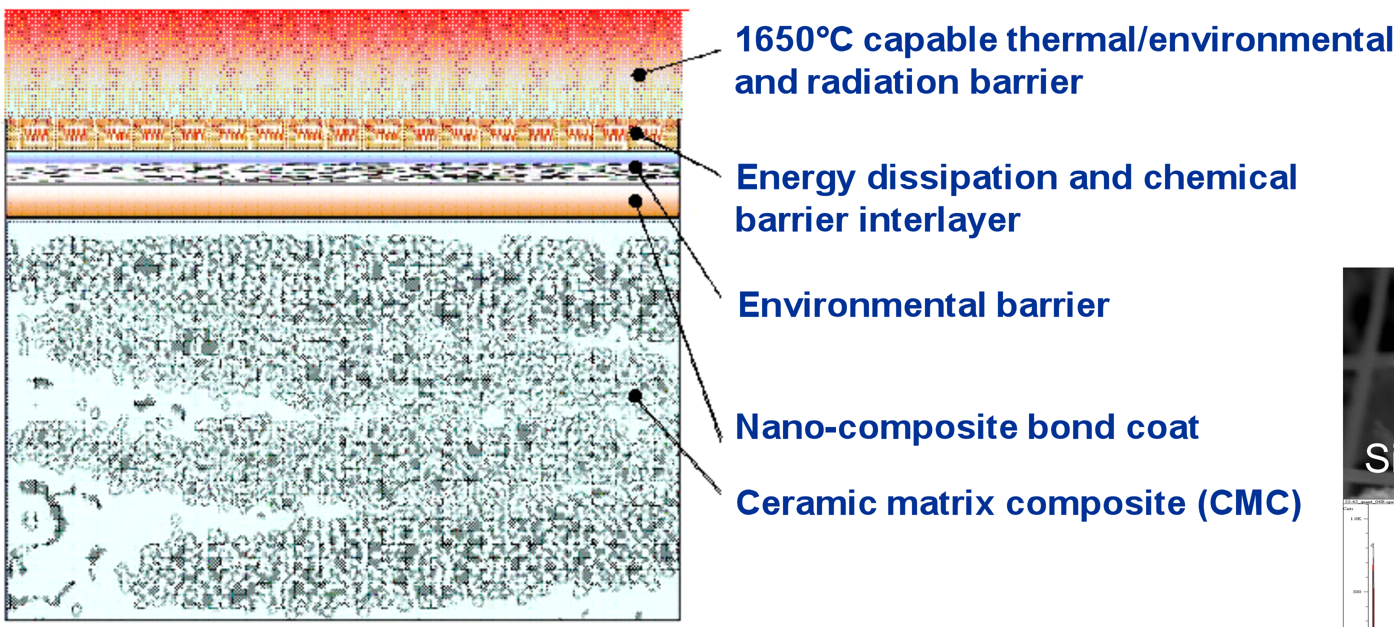
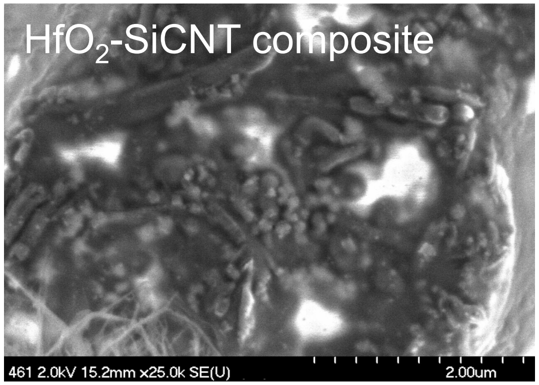
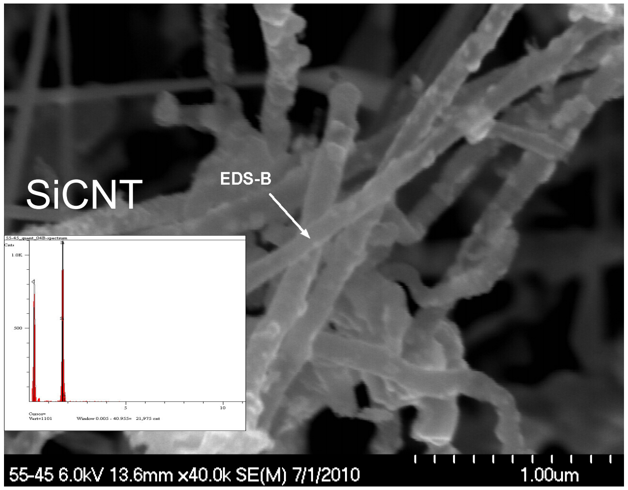
The 35th International Conference on Advanced Ceramics and Composites
Daytona Beach, FL
January 23-28,2011

Introduction

- Environmental barrier coating (EBC) systems are used for protecting Si-based ceramic hot section components
- Nanotube composites, having extremely high stiffness and strength and functional properties, are currently being considered for EBC to improve the coating performance
- In particular, SiC nanotubes (SiCNTs) are being incorporated into EBC bond coats to increase their strength and toughness

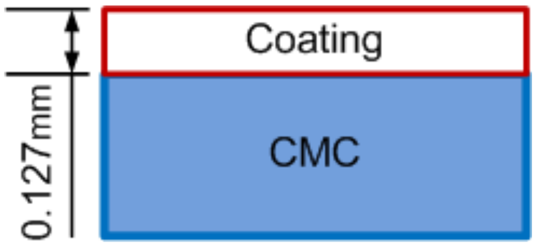






Advantages of Nanotube Reinforcements

Nanotubes as compared to other micro scale reinforcements:



Vf=20%	Fiber	Wisker	Nanotube
r =	20 μm	1~5 μm	0.005~0.1 μm
Spacing	25 μm	1.3~6.5 μm	0.0065~0.130 μm
#	2~3	8~50	800~4000

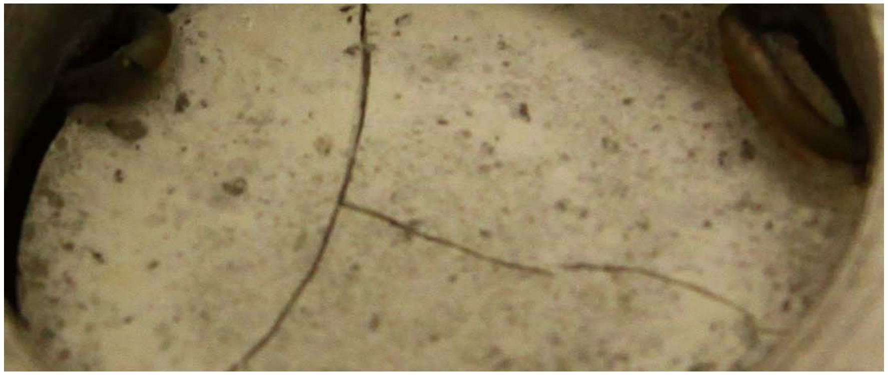
- Can achieve much higher volume fraction
- More crack arresters due to more interfaces
- Exhibit more homogenized material response
- Less stress concentration (Gradual stress distribution)

Improvement of toughness with SiCNT

HfO_2-SiCNT nano-composites, tested at 1450˚C (ΔT=1000˚C), with Random orientation SiCNT , Wavy, 5 μm long:

HfO_2 + 0% SiCNT:

HfO_2 + 20% SiCNT:



HfO_2 + 40% SiCNT

- Higher volume fraction showed improved toughness/strength

Outline

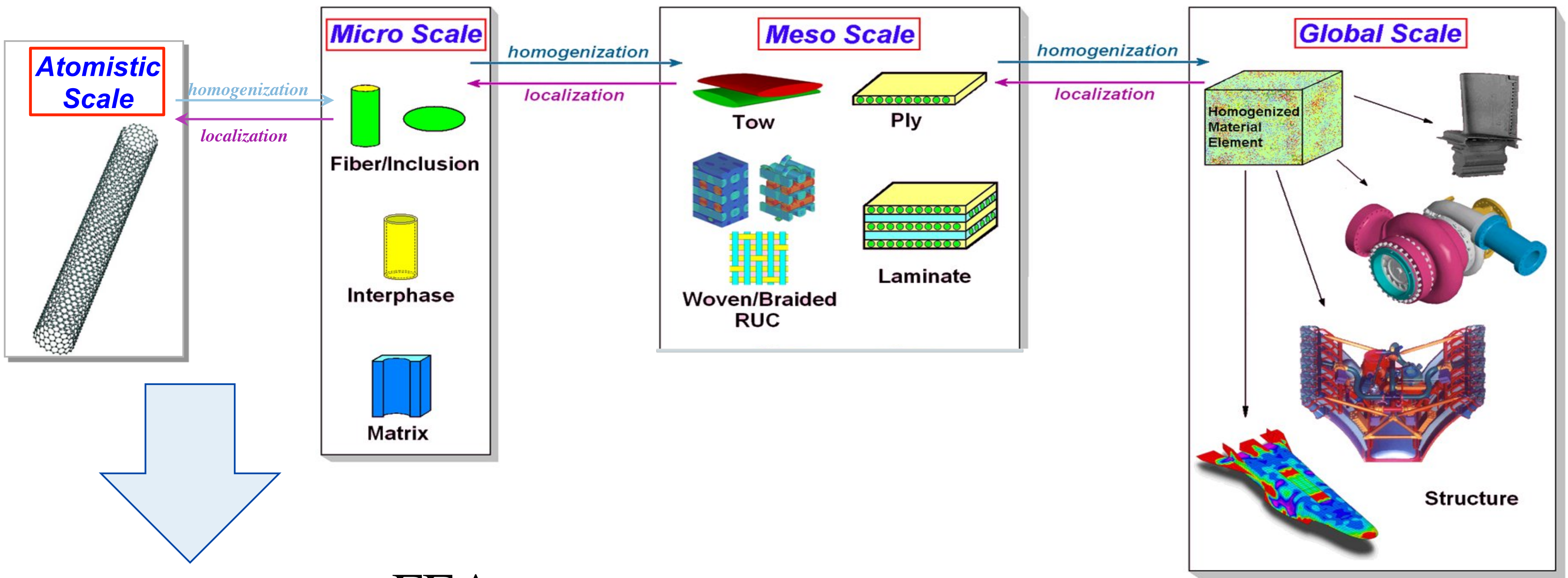
To understand mechanical improvement in toughness/strength

- Multiscale modeling approach for nano-composite property determination:
    - HfO_2 + SiCNT nano-composite model system
- FEA to determine micro (nano) scale properties
- Homogenization technique – Micromechanics Analysis Code (MAC/GMC)
- Results and discussions on effect of SiCNT architectures
- Summary

Approach to Determine Global Scale Mechanical Properties

$K = \sigma (\pi a)^{1/2}$, where $\sigma = f(\mathbf{E}, \Delta\mathbf{T}, \ldots.)$

- Increasing stiffness E will improve toughness K for a given material system
- Multi-scale modeling approach is used to determine bulk composite stiffness



- V_f
- Length
- Waviness
- Orientation

FEA

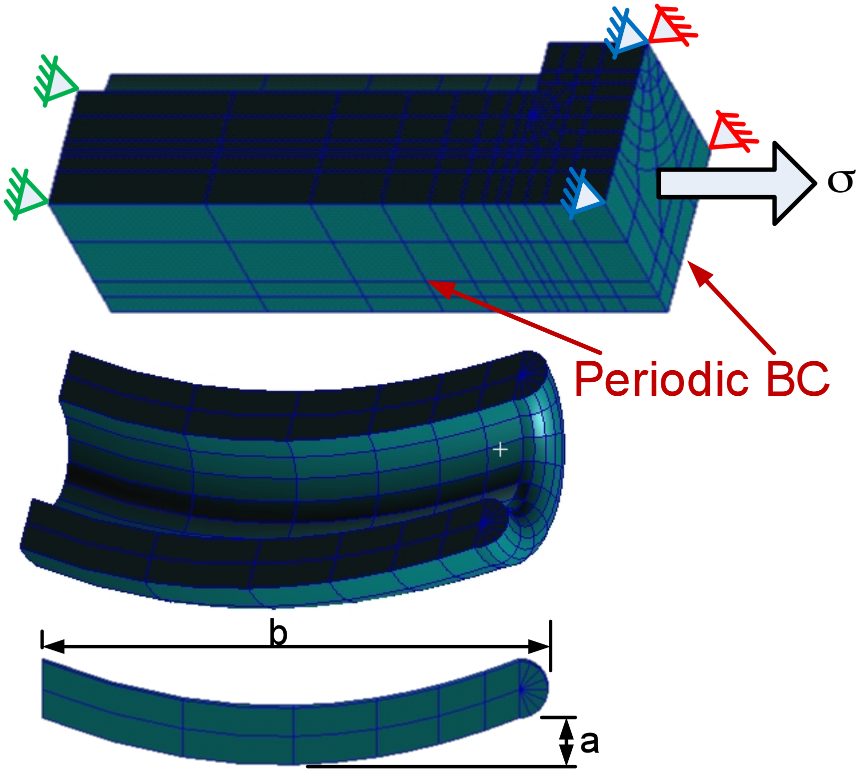
MAC/GMC

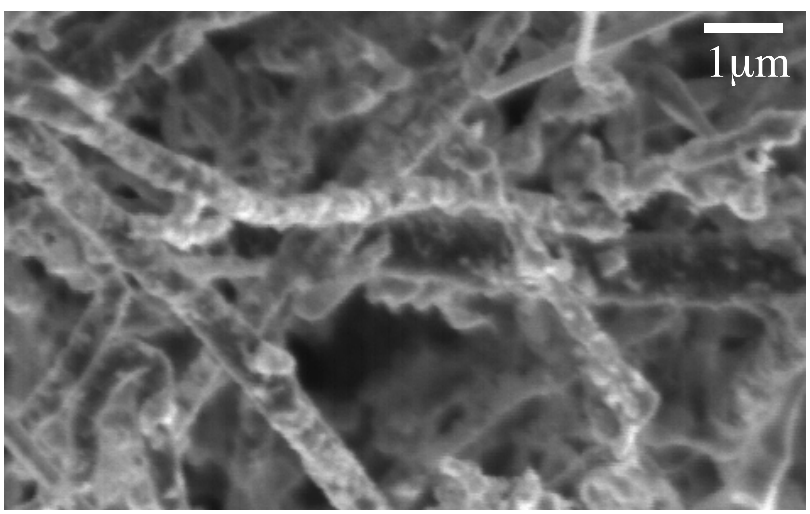
Various Micro/Meso scale RVEs

MAC/GMC

Global scale Mechanical properties

FEA Simulation (Micro scale properties)





- Assuming perfect bond and equally distributed
- SiCNT: E_{NT} = 600GPa, ν = 0.3
- HfO_2 Matrix: E_M = 100 GPa , ν = 0.3
- SiCNT radius: r = 0.05 μm (50 nm)
- SiCNT length: L = 0.5, 1, 5, 10 ,50 μm (r/L=10, 20, 100, 200, 1000)
- Waviness: λ = a/b = 0.0, 0.1, 0.2
- Orientation: θ = 0, 30, 45, 60, 90°
- Volume fraction: V_f = 0~ 60 %

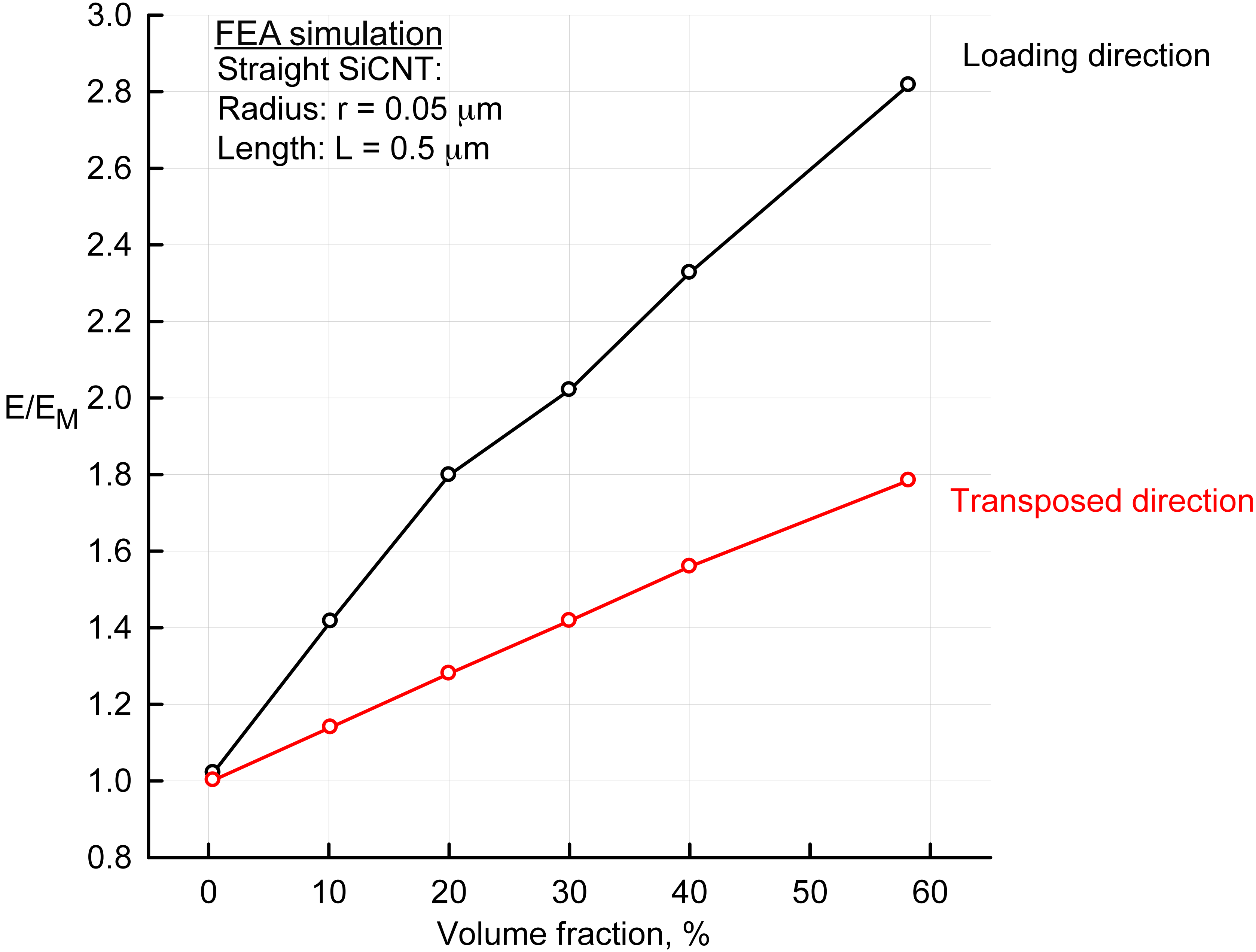
FEA model:

Element Type: Hex20 and Wedge15

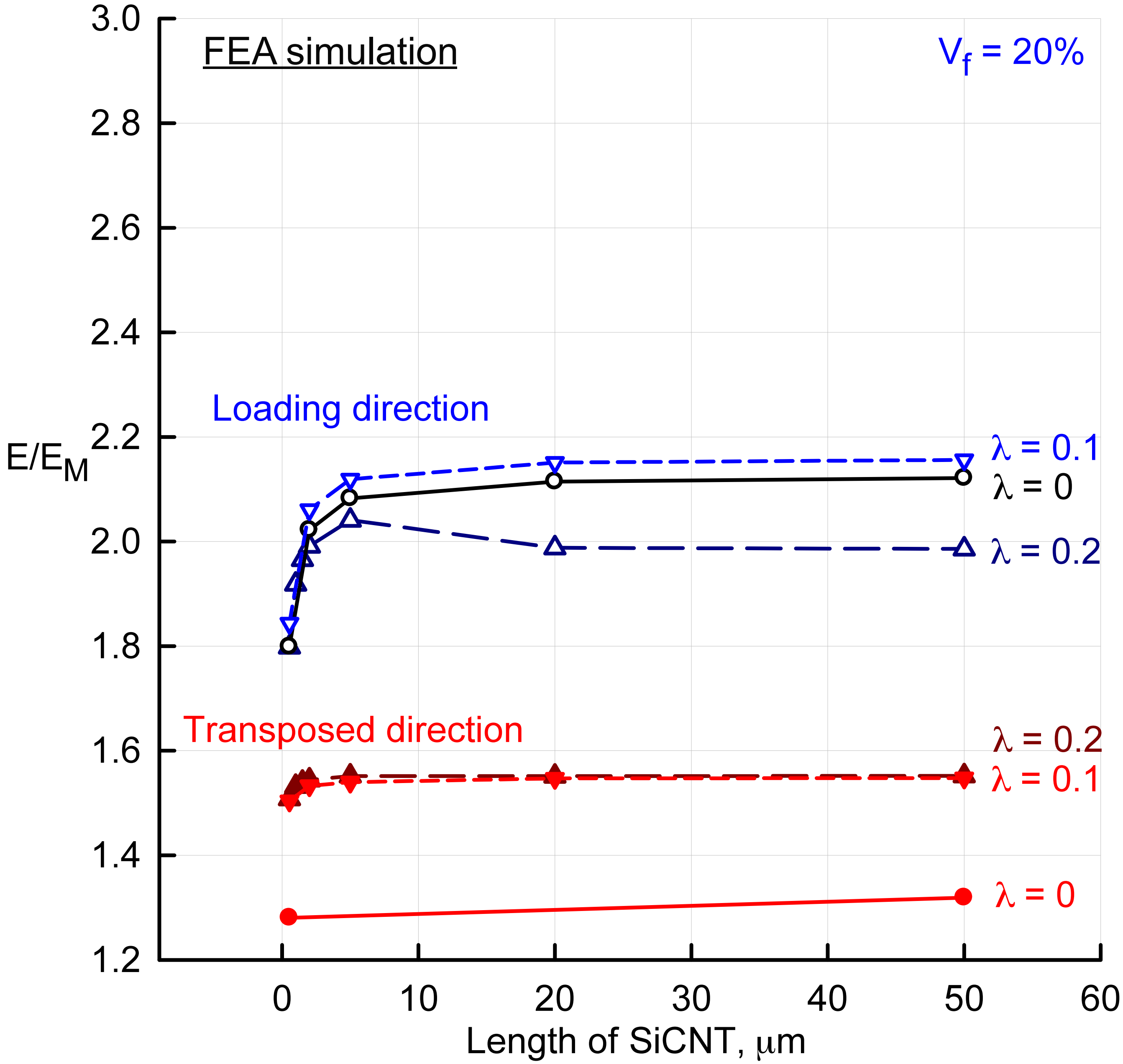
# of Nodes: 3000 ~ 90000

# of Elements: 400 ~ 15000

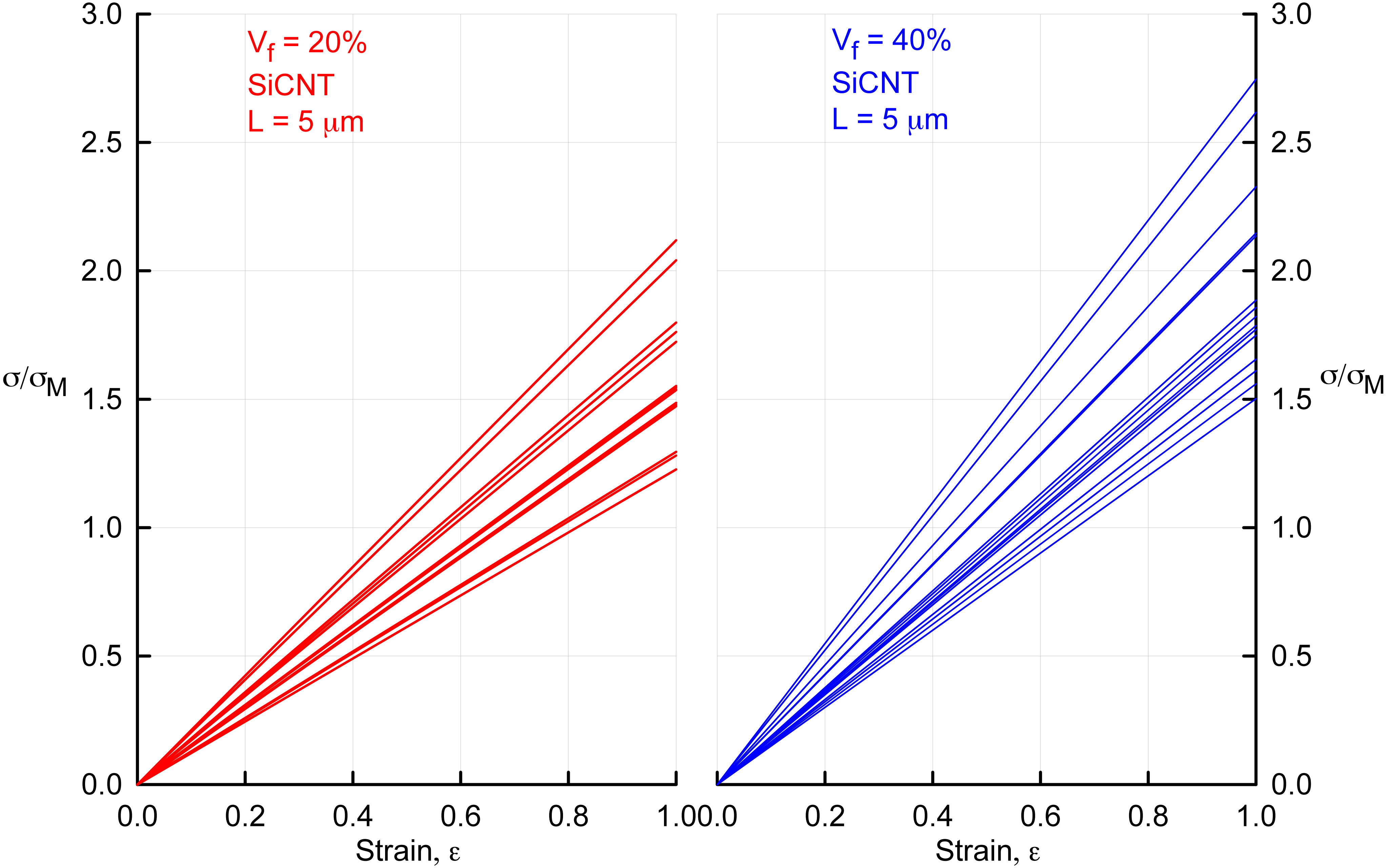
Micro Scale Properties: V_f and Length effect



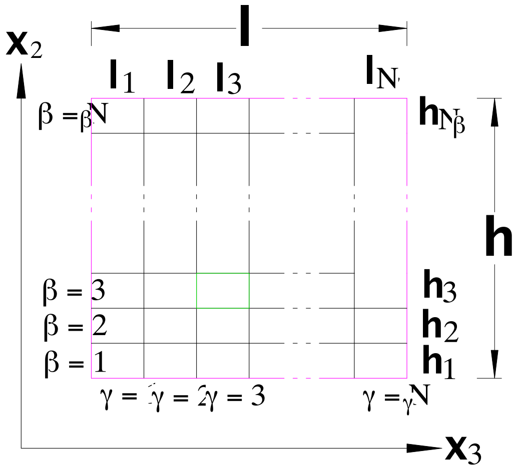
Micro Scale Properties: Effect of Waviness



Micro Scale Properties: Summary(FEA simulation)



Homogenization (Micro to Macro by MAC/GMC)



Double Periodicity

x1

Triple Periodicity

- **1st order Taylor series of displacement field**
- **Satisfy continuity of displacements & tractions between subcells**
- **Impose periodicity conditions on displacements and tractions at the unit cell boundaries**

✓**Macro-level Constitutive Equations**

$$\bar{\sigma} = B^{*}(\bar{\varepsilon} - \bar{\varepsilon}^{I} + \bar{\varepsilon}^{T})$$

Provides effective constitutive equation for composite material

$$B^{*} = \frac{1}{dhl}\sum_{\alpha=1}^{N_\alpha}\sum_{\beta=1}^{N_\beta}\sum_{\gamma=1}^{N_\gamma} d_\alpha h_\beta l_\gamma C^{(\alpha\beta\gamma)} A^{(\alpha\beta\gamma)}$$

$$\bar{\varepsilon}^{I} = \frac{-B^{*-1}}{dhl}\sum_{\alpha=1}^{N_\alpha}\sum_{\beta=1}^{N_\beta}\sum_{\gamma=1}^{N_\gamma} d_\alpha h_\beta l_\gamma C^{(\alpha\beta\gamma)}(D^{(\alpha\beta\gamma)}\varepsilon_S^{I} - \bar{\varepsilon}^{I(\alpha\beta\gamma)})$$

$$\bar{\varepsilon}^{T} = \frac{-B^{*-1}}{dhl}\sum_{\alpha=1}^{N_\alpha}\sum_{\beta=1}^{N_\beta}\sum_{\gamma=1}^{N_\gamma} d_\alpha h_\beta l_\gamma C^{(\alpha\beta\gamma)}(D^{(\alpha\beta\gamma)}\varepsilon_S^{T} - \bar{\varepsilon}^{T(\alpha\beta\gamma)})$$

✓**Micro-level Field Equations (subcell)**

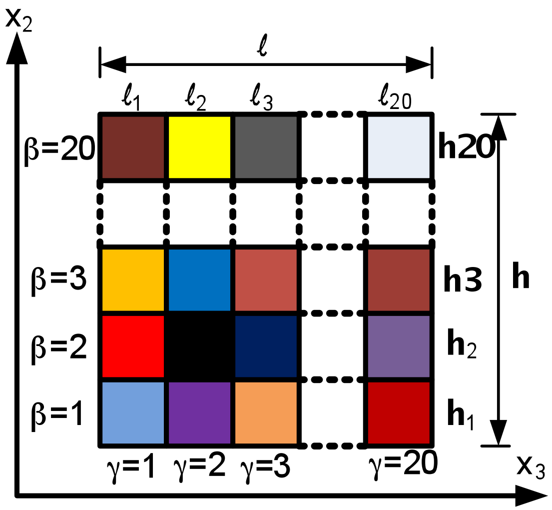
$$\bar{\varepsilon}^{(\alpha\beta\gamma)} = A^{(\alpha\beta\gamma)}\bar{\varepsilon} + D^{(\alpha\beta\gamma)}(\varepsilon_S^{I} + \varepsilon_S^{T})$$

$$\bar{\sigma}^{(\alpha\beta\gamma)} = C^{(\alpha\beta\gamma)}[A^{(\alpha\beta\gamma)}\bar{\varepsilon} + D^{(\alpha\beta\gamma)}(\varepsilon_S^{I} + \varepsilon_S^{T}) - (\bar{\varepsilon}^{I(\alpha\beta\gamma)} + \bar{\varepsilon}^{T(\alpha\beta\gamma)})]$$

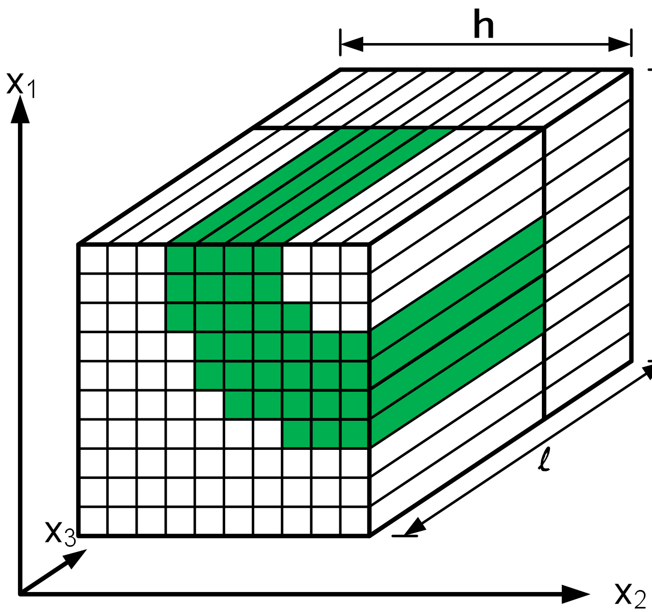
Provides access to local stresses and strains in fiber and matrix

Paley & Aboudi 1992, Aboudi 1995, Pindera & Bednarcyk 1999

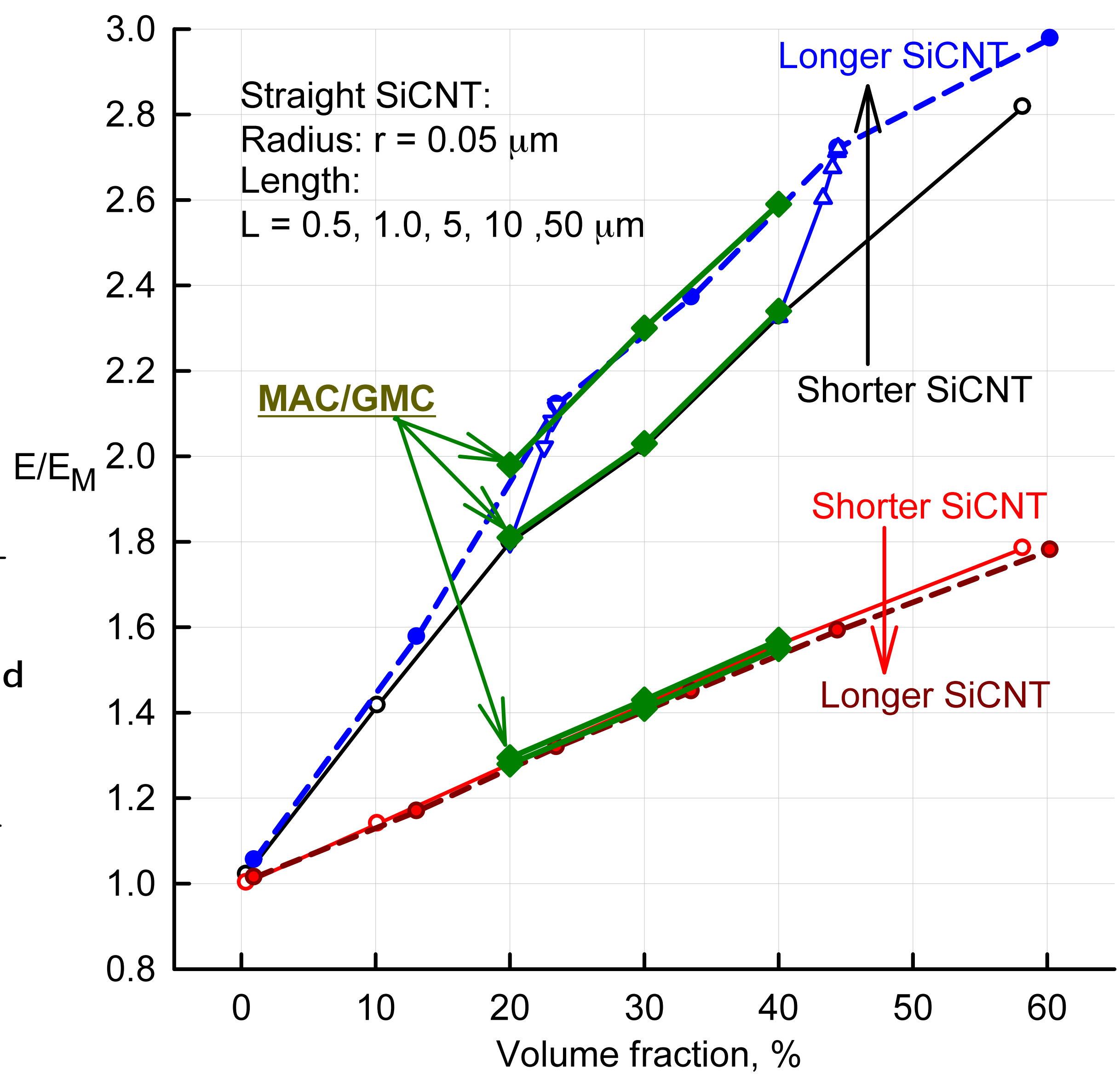
Homogenization (Micro to Macro by MAC/GMC)



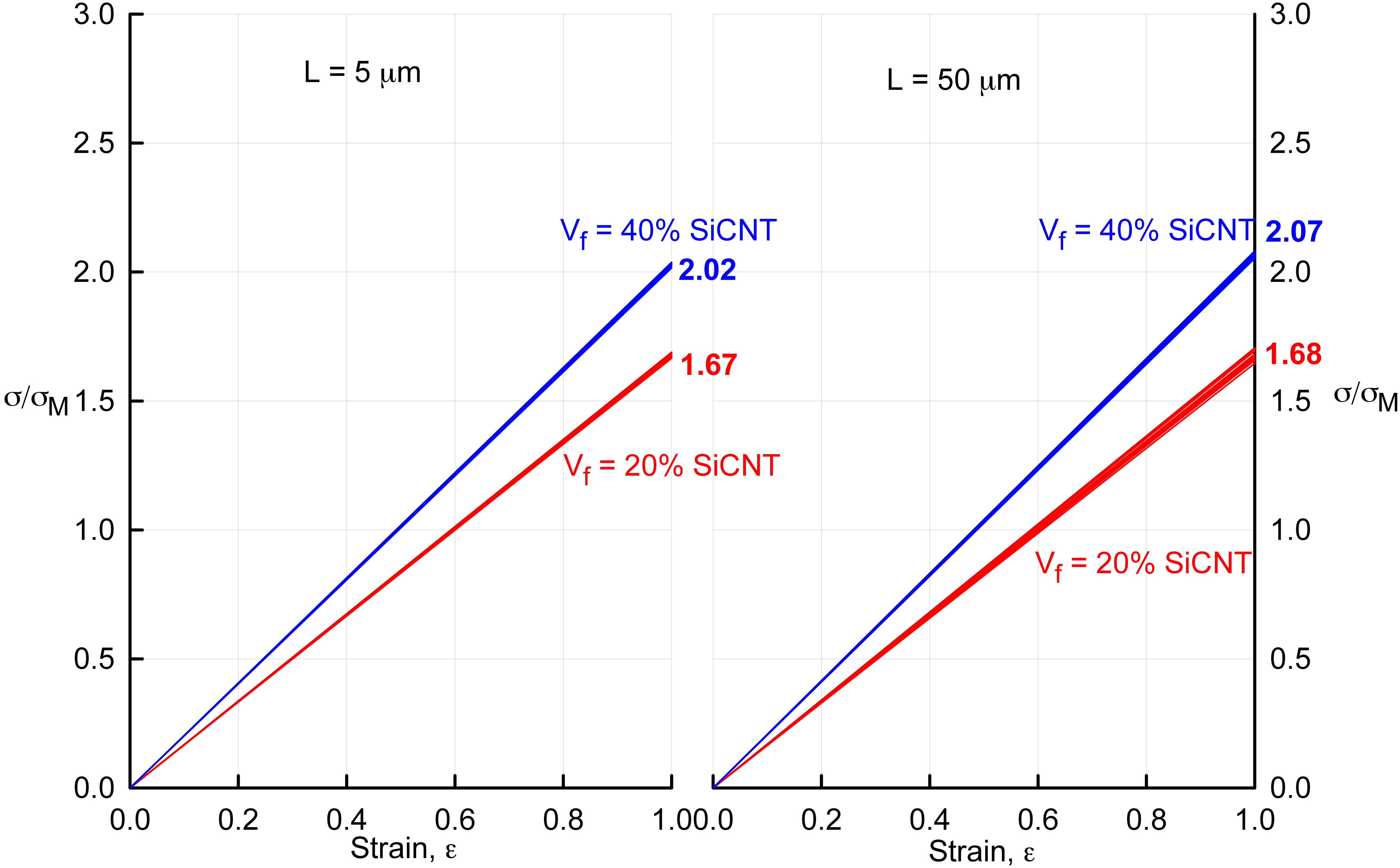
Double Periodicity



Triple Periodicity



Macro Scale Properties for SiCNT Composites



Improvement of toughness with SiCNT

HfO_2-SiCNT nano-composites, tested at 1450˚C (ΔT=1000˚C), with Random orientation SiCNT , Wavy, 5 μm long:

$K = \sigma (\pi a)^{1/2}$, where $\sigma = f(\mathbf{E}, \mathbf{\Delta T}, \ldots)$

HfO_2 + 0% SiCNT:

$E = E_m = 100$ GPa

HfO_2 + 20% SiCNT:

$E = 1.67\sim1.68\ E_m$

Toughness improvement: less than +67~68 %

HfO_2 + 40% SiCNT:

$E = 2.02\sim2.07\ E_m$

Toughness improvement: more than +102~107 %

Summary

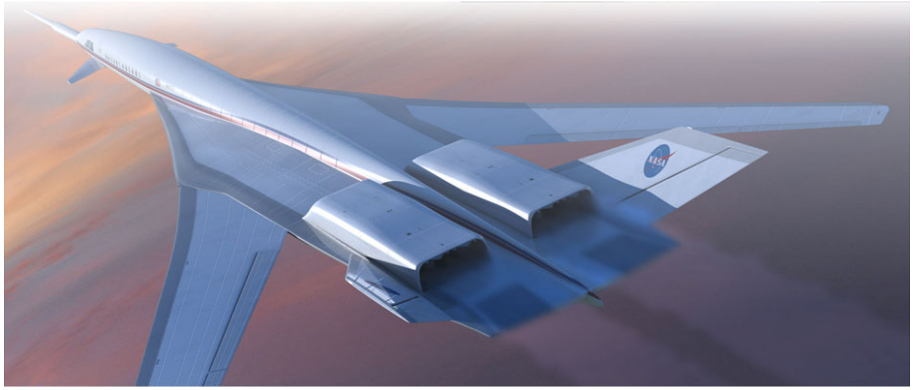
- Based on micromechanics modeling, relative improvement in toughness was investigated.
- V_f of 20~40% showed optimum improvement in material properties
- Waviness tends to improve transverse stiffness
- r/L (NT radius to length) ratio > 100 showed no improvement in stiffness
- Totally random orientation with wavy and straight NT provided Isotropic material behavior
- Based on preliminary experiments, in order to prevent from surface cracking, 40% V_f of SiCNT (+102% toughness improvement) is needed and 20% V_f (+67% toughness improvement) was not sufficient

Future Work

- Conduct classical fracture test (3pt bend specimen) and indentation test to measure fracture toughness
- Determine SiCNT strength and interfacial bonding strength from Molecular dynamics (MD) simulation

Acknowledgement

The work was supported by NASA Fundamental Aeronautics Program (FAP) **Supersonics** Project.



NASA Supersonics